

=> fil reg

FILE 'REGISTRY' ENTERED AT 15:59:22 ON 24 JUL 2006  
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=> d his

(FILE 'HOME' ENTERED AT 14:26:04 ON 24 JUL 2006)

FILE 'HCAPLUS' ENTERED AT 14:26:17 ON 24 JUL 2006  
 E US20050261207/PN

L1 1 S E3  
 SEL RN

FILE 'REGISTRY' ENTERED AT 14:27:33 ON 24 JUL 2006

L2 32 S E1-32  
 L3 STR  
 L4 0 S L3  
 L5 STR L3  
 L6 5 S L5  
 L7 STR L5  
 L8 5 S L7  
 L9 138 S L7 FUL  
 SAV L9 ISS601/A  
 L10 14 S L2 AND L9

FILE 'HCAPLUS' ENTERED AT 15:32:17 ON 24 JUL 2006

L11 908 S L9  
 L12 1 S L10

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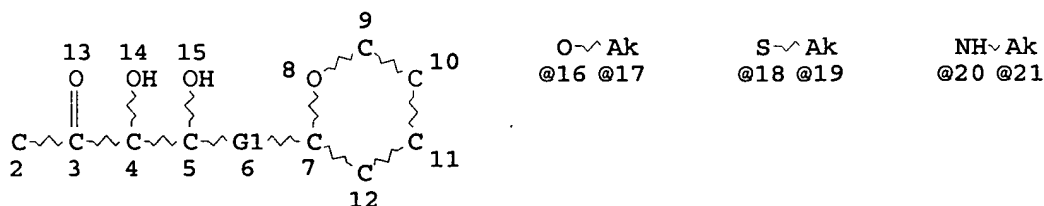
L17 7 S L16

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L7 STR



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NODE ATTRIBUTES:

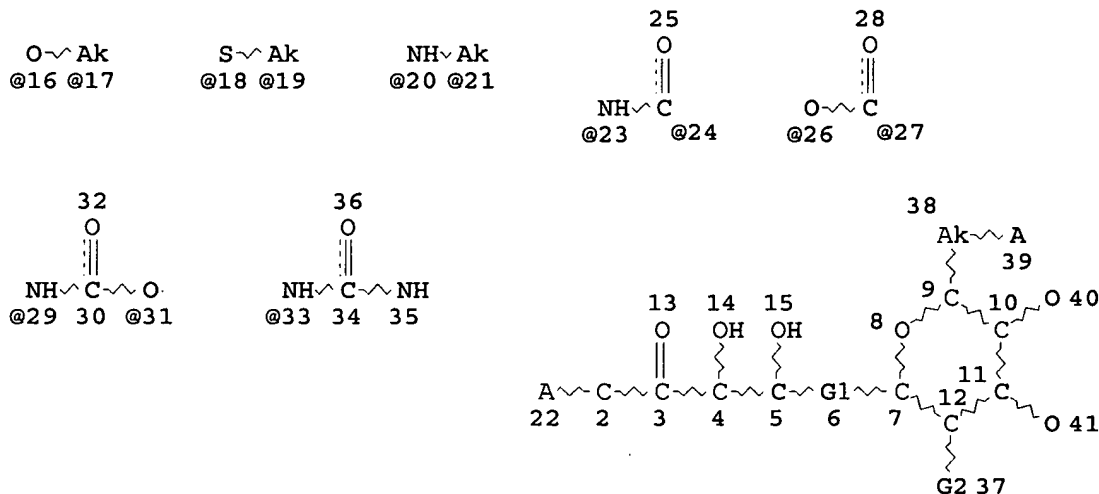
DEFAULT MLEVEL IS ATOM

GGCAT IS SAT AT 17

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE  
L9 138 SEA FILE=REGISTRY SSS FUL L7  
L15 STR



VAR G1=O/16-5 17-7/S/18-5 19-7/NH/20-5 21-7/17-5 16-7/18-7 19-5/20-7 21-5  
VAR G2=O/NH/23/24/26/27/29/31/33

NODE ATTRIBUTES:  
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DEFAULT MLEVEL IS ATOM  
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GGCAT IS SAT AT 38  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 40

STEREO ATTRIBUTES: NONE  
L16 19 SEA FILE=REGISTRY SUB=L9 SSS FUL L15

100.0% PROCESSED 132 ITERATIONS 19 ANSWERS  
SEARCH TIME: 00.00.01

=> fil hcap  
FILE 'HCAPLUS' ENTERED AT 16:00:42 ON 24 JUL 2006  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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 COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

=> d l17 ibib abs hitstr hitind 1-7

L17 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:333730 HCAPLUS  
 DOCUMENT NUMBER: 140:332537  
 TITLE: Glucose-based compounds with affinity to  
 P-selectin  
 INVENTOR(S): Appeldoorn, Chantal Catharina Maria; Biessen,  
 Erik Anna Leonardus; Molenaar, Thomas Jacobus  
 Maria; Van Berkel, Theodorus Josephus Cornelis  
 PATENT ASSIGNEE(S): Yamanouchi Europe B.V., Neth.  
 SOURCE: PCT Int. Appl., 28 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004033473	A1	20040422	WO 2003-EP11457	20031013
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2501842	AA	20040422	CA 2003-2501842	20031013
AU 2003278090	A1	20040504	AU 2003-278090	20031013
EP 1549658	A1	20050706	EP 2003-769400	20031013
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003015231	A	20050823	BR 2003-15231	20031013
JP 2006503876	T2	20060202	JP 2004-542495	20031013
US 2005261207	A1	20051124	US 2005-530601	20050407

PRIORITY APPLN. INFO.:

EP 2002-79232

A

200210  
11

WO 2003-EP11457

W

200310  
13

OTHER SOURCE(S): MARPAT 140:332537

AB The invention relates to certain glucose-based compds. with affinity to P-selectin to act as antagonists or partial antagonists of P-selectin. These compds. are useful as targeting ligands with an ability to target drugs and genetic material to cells and tissues expressing P-selectin. The synthesis of glucose-based compds. and their use for the prepn. of pharmaceutical compns. for the treatment of P-selectin-assocd. disorders, the conjugates, pharmaceutical carriers and drug delivery systems comprising these compds., and a method for detg. whether a compd. is capable of binding to P-selectin are also described.

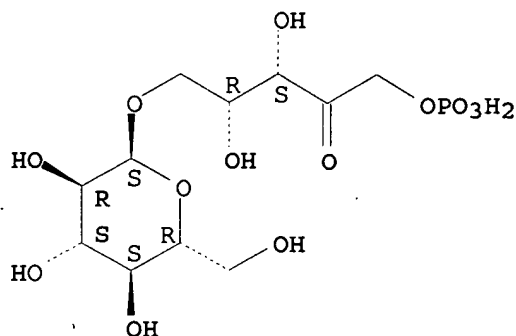
IT 681121-09-5P 681121-11-9P 681121-12-0P  
681121-13-1P 681121-25-5P 681121-26-6P  
681121-27-7P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of glucose-based compds. with affinity to P-selectin)

RN 681121-09-5 HCAPLUS

CN D-threo-2-Pentulose, 5-O- $\alpha$ -D-glucopyranosyl-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

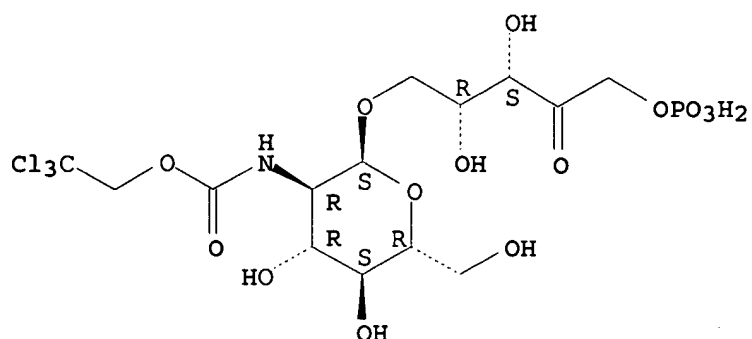
Absolute stereochemistry.



RN 681121-11-9 HCAPLUS

CN D-threo-2-Pentulose, 5-O-[2-deoxy-2-[(2,2,2-trichloroethoxy)carbonyl]amino]- $\alpha$ -D-glucopyranosyl-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

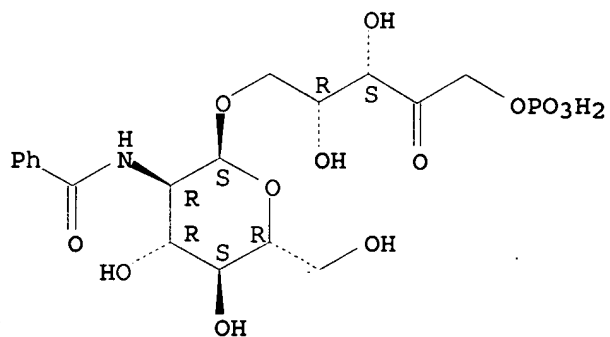
Absolute stereochemistry.



RN 681121-12-0 HCAPLUS

CN D-threo-2-Pentulose, 5-O-[2-(benzoylamino)-2-deoxy- $\alpha$ -D-glucopyranosyl]-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

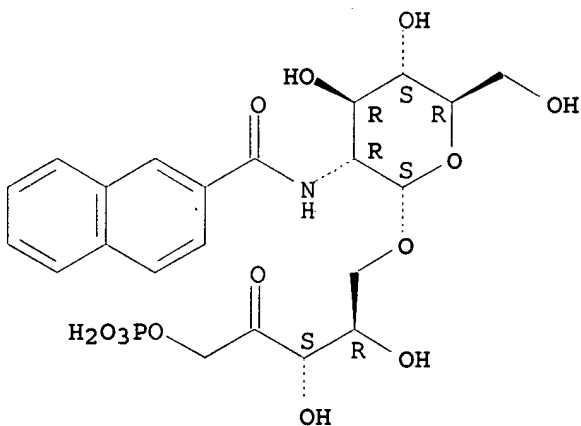
Absolute stereochemistry.



RN 681121-13-1 HCAPLUS

CN D-threo-2-Pentulose, 5-O-[2-deoxy-2-[(2-naphthalenylcarbonyl)amino]- $\alpha$ -D-glucopyranosyl]-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

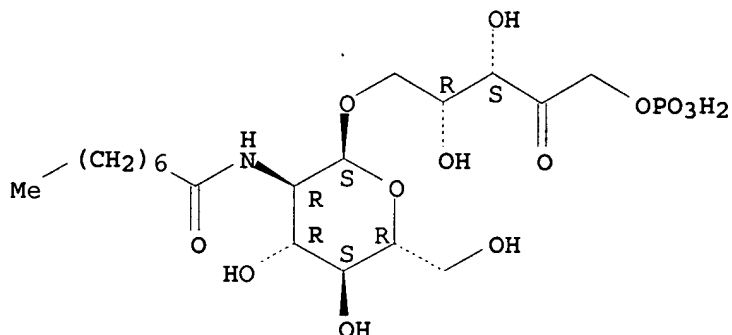
Absolute stereochemistry.



RN 681121-25-5 HCAPLUS

CN D-threo-2-Pentulose, 5-O-[2-deoxy-2-[(1-oxooctyl)amino]- $\alpha$ -D-glucopyranosyl]-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

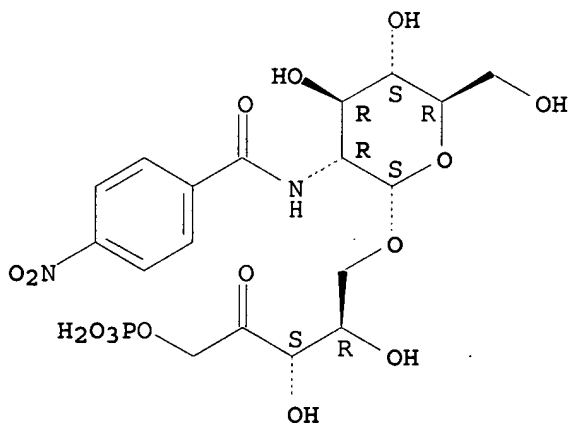
Absolute stereochemistry.



RN 681121-26-6 HCAPLUS

CN D-threo-2-Pentulose, 5-O-[2-deoxy-2-[(4-nitrobenzoyl)amino]- $\alpha$ -D-glucopyranosyl]-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

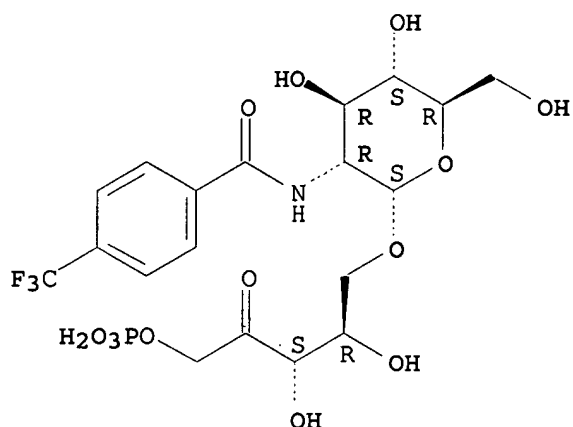
Absolute stereochemistry.



RN 681121-27-7 HCAPLUS

CN D-threo-2-Pentulose, 5-O-[2-deoxy-2-[[4-(trifluoromethyl)benzoyl]amino]- $\alpha$ -D-glucopyranosyl]-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



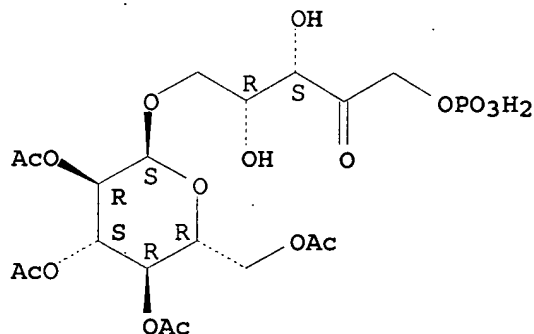
IT 681121-10-8P 681121-19-7P 681121-20-0P  
 681121-21-1P 681121-22-2P 681121-23-3P  
 681121-24-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (prepn. of glucose-based compds. with affinity to P-selectin)

RN 681121-10-8 HCAPLUS

CN D-threo-2-Pentulose, 5-O-(2,3,4,6-tetra-O-acetyl- $\alpha$ -D-glucopyranosyl)-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

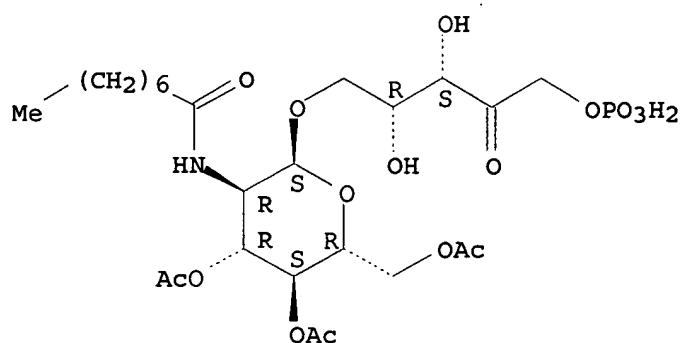
Absolute stereochemistry.



RN 681121-19-7 HCAPLUS

CN D-threo-2-Pentulose, 5-O-[3,4,6-tri-O-acetyl-2-deoxy-2-[(1-oxooctyl)amino]- $\alpha$ -D-glucopyranosyl]-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

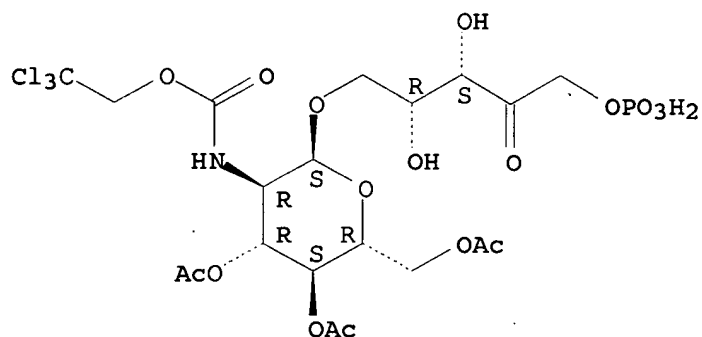
Absolute stereochemistry.



RN 681121-20-0 HCAPLUS

CN D-threo-2-Pentulose, 5-O-[3,4,6-tri-O-acetyl-2-deoxy-2-[(2,2,2-trichloroethoxy) carbonyl] amino]- $\alpha$ -D-glucopyranosyl]-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

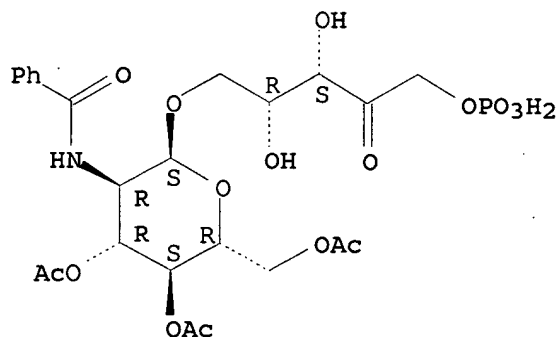
Absolute stereochemistry.



RN 681121-21-1 HCAPLUS

CN D-threo-2-Pentulose, 5-O-[3,4,6-tri-O-acetyl-2-(benzoylamino)-2-deoxy- $\alpha$ -D-glucopyranosyl]-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

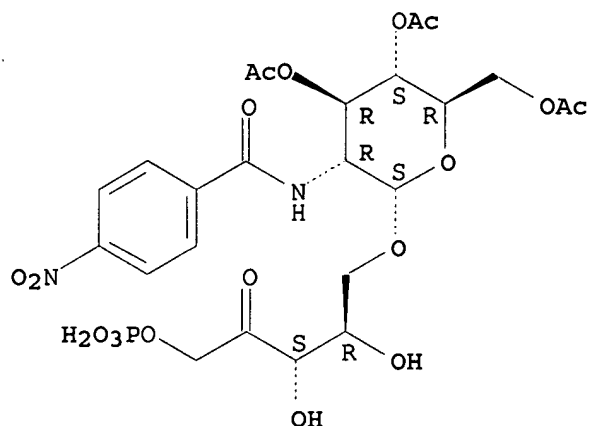


RN 681121-22-2 HCAPLUS

CN D-threo-2-Pentulose, 5-O-[3,4,6-tri-O-acetyl-2-deoxy-2-[(4-nitrobenzoyl) amino]- $\alpha$ -D-glucopyranosyl]-, 1-(dihydrogen

phosphate) (9CI) (CA INDEX NAME)

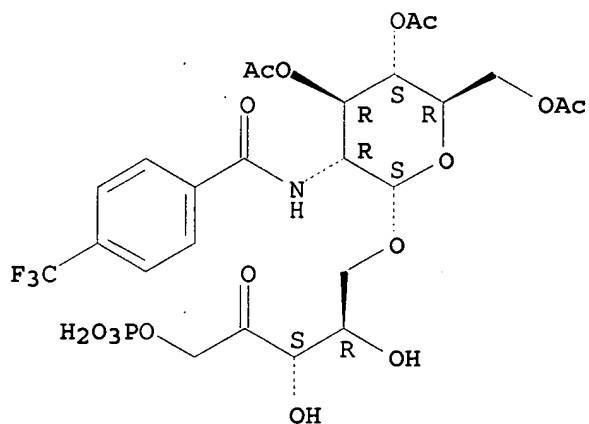
Absolute stereochemistry.



RN 681121-23-3 HCAPLUS

CN D-threo-2-Pentulose, 5-O-[3,4,6-tri-O-acetyl-2-deoxy-2-[[4-(trifluoromethyl)benzoyl]amino]-α-D-glucopyranosyl]-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

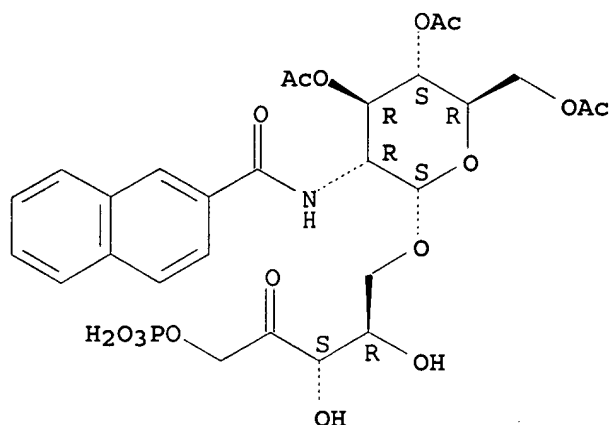
Absolute stereochemistry.



RN 681121-24-4 HCAPLUS

CN D-threo-2-Pentulose, 5-O-[3,4,6-tri-O-acetyl-2-deoxy-2-[(2-naphthalenylcarbonyl)amino]-α-D-glucopyranosyl]-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H015-04  
ICS A61K031-70; A61P029-00  
CC 1-12 (Pharmacology)  
Section cross-reference(s): 33, 63  
IT 681121-09-5P 681121-11-9P 681121-12-0P  
681121-13-1P 681121-25-5P 681121-26-6P  
681121-27-7P  
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of glucose-based compds. with affinity to P-selectin)  
IT 39698-55-0P 97562-23-7P 131474-49-2P 151557-75-4P  
681121-10-8P 681121-14-2P 681121-15-3P 681121-16-4P  
681121-17-5P 681121-18-6P 681121-19-7P  
681121-20-0P 681121-21-1P 681121-22-2P  
681121-23-3P 681121-24-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. of glucose-based compds. with affinity to P-selectin)  
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1999:521766 HCAPLUS  
DOCUMENT NUMBER: 131:306669  
TITLE: Selectin/Glycoconjugate Binding Assays for the Identification and Optimization of Selectin Antagonists  
AUTHOR(S): Weitz-Schmidt, Gabriele; Gong, Ke Wei; Wong, Chi-Huey  
CORPORATE SOURCE: Transplantation Research, Novartis Pharma A.G., Basel, CH-4002, Switz.  
SOURCE: Analytical Biochemistry (1999), 273(1), 81-88  
CODEN: ANBCA2; ISSN: 0003-2697  
PUBLISHER: Academic Press  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB In this study we describe ELISA-type P- and L-selectin binding assays for the anal. of selectin antagonists. A biotinylated polyacrylamide-type glycoconjugate contg. sialyl Lewis A (sLea-polymer) is utilized as a synthetic ligand for both selectins

analogous to the E-selectin assay we have developed recently. Following precomplexation of sLea-polymer with streptavidin-peroxidase, the complex is added to microtiter plates coated with the recombinant selectins. Binding of sLea-polymer to the immobilized selectins is measured by the peroxidase reaction. SLea-polymer was found to bind to P- and L-selectin in a cation-dependent manner. The interaction of the polymer was blocked by neutralizing anti-P- and anti-L-selectin antibody, resp. The ref. compds. heparin and fucoidan inhibited binding in both assays. Sialyl Lewis X (sLex) blocked binding to L-selectin by 46% at 3 mM, whereas no inhibition was obsd. in the P-selectin assay up to 3 mM. Control polymers contg. sialic acid or  $\beta$ -d-glucose instead of sLea weakly bound or failed to bind to the selectins. Both assays are rapid to perform and of low variability. The P-selectin assay was successfully employed to identify and optimize novel carbohydrate-based P-selectin antagonists. The P-, L-, and E-selectin assays were used to det. the fine selectivity of several sLex-related selectin antagonists. These studies together suggest that sLea-polymer-based selectin assays are well suited for primary screening and the characterization of selectin antagonists. (c) 1999 Academic Press.

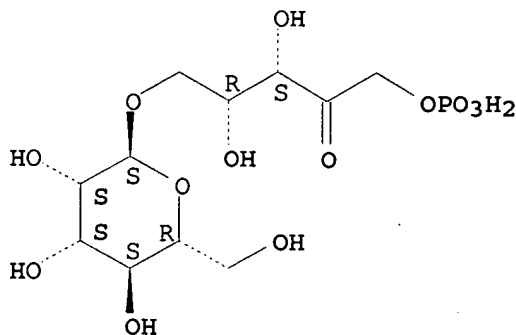
IT 194980-01-3, FM 233

RL: ANT (Analyte); ANST (Analytical study)  
(selectin/glycoconjugate binding assays for identification and optimization of selectin antagonists)

RN 194980-01-3 HCAPLUS

CN D-threo-2-Pentulose, 5-O- $\alpha$ -D-mannopyranosyl-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 1-1 (Pharmacology)

Section cross-reference(s): 15

IT 194980-01-3, FM 233

RL: ANT (Analyte); ANST (Analytical study)  
(selectin/glycoconjugate binding assays for identification and optimization of selectin antagonists)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE  
FOR THIS RECORD. ALL CITATIONS AVAILABLE  
IN THE RE FORMAT

L17 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

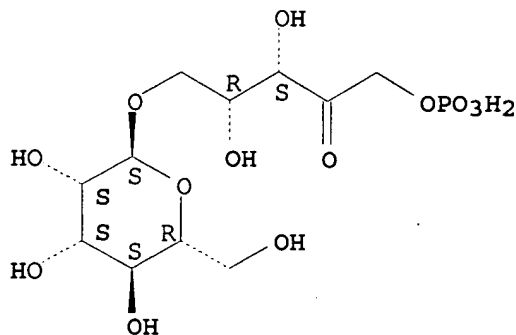
ACCESSION NUMBER: 1999:235765 HCAPLUS

DOCUMENT NUMBER: 130:296935

TITLE: Synthesis of sialyl Lewis x mimetics as selectin inhibitors by enzymic aldol condensation

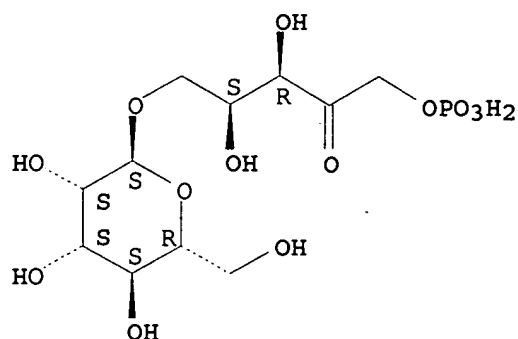
reactions  
 AUTHOR(S): Lin, Chun-Cheng; Moris-Varas, Francisco;  
 Weitz-Schmidt, Gabriel; Wong, Chi-Huey  
 CORPORATE SOURCE: Department of Chemistry and Skaggs Institute of  
 Chemical Biology, The Scripps Research  
 Institute, La Jolla, CA, 92037, USA  
 SOURCE: Bioorganic & Medicinal Chemistry (1999), 7(3),  
 425-433  
 CODEN: BMECEP; ISSN: 0968-0896  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Sialic acids were prepd. as antiinflammatory agents and E-, L-, and  
 P-selectin inhibitors. Several D-mannosyl phosphate/phosphonate  
 derivs. have been enzymically prepd. as sialyl Lewis x  
 tetrasaccharide mimics, which showed strong-to-moderate inhibition  
 against E-, P-, and L-selectins. The synthesis of these mimics is  
 very straightforward; mannosyl aldehyde derivs. are condensed with  
 dihydroxyacetone phosphate (DHAP) in the presence of a  
 DHAP-dependent aldolase to provide mannosyl phosphates.  
 IT 194980-01-3  
 RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); BIOL (Biological study)  
 (synthesis of sialyl Lewis x mimetics as selectin inhibitors by  
 enzymic aldol condensation reactions)  
 RN 194980-01-3 HCAPLUS  
 CN D-threo-2-Pentulose, 5-O- $\alpha$ -D-mannopyranosyl-, 1-(dihydrogen  
 phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 223121-83-3P 223121-90-2P 223121-97-9P  
 RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); BIOL  
 (Biological study); PREP (Preparation)  
 (synthesis of sialyl Lewis x mimetics as selectin inhibitors by  
 enzymic aldol condensation reactions)  
 RN 223121-83-3 HCAPLUS  
 CN L-threo-2-Pentulose, 5-O- $\alpha$ -D-mannopyranosyl-, 1-(dihydrogen  
 phosphate) (9CI) (CA INDEX NAME)

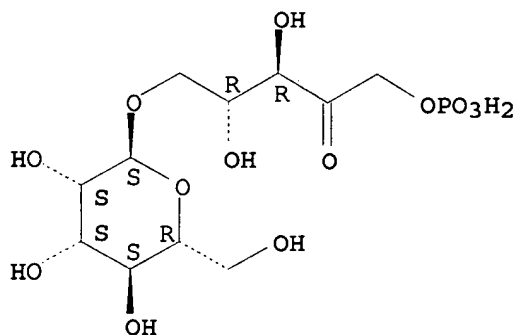
Absolute stereochemistry.



RN 223121-90-2 HCAPLUS

CN D-erythro-2-Pentulose, 5-O-α-D-mannopyranosyl-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

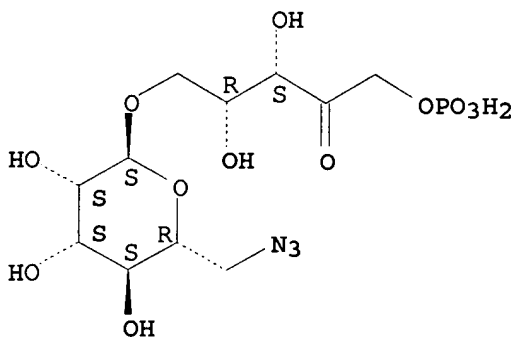
Absolute stereochemistry.



RN 223121-97-9 HCAPLUS

CN D-threo-2-Pentulose, 5-O-(6-azido-6-deoxy-α-D-mannopyranosyl)-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 33-8 (Carbohydrates)

Section cross-reference(s): 1, 15

IT 194980-01-3 194980-02-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(synthesis of sialyl Lewis x mimetics as selectin inhibitors by enzymic aldol condensation reactions)

IT 223121-83-3P 223121-90-2P 223121-97-9P

223122-03-0P 223122-14-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis of sialyl Lewis x mimetics as selectin inhibitors by enzymic aldol condensation reactions)

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:293511 HCAPLUS

DOCUMENT NUMBER: 129:4814

TITLE: Preparation of sialyl Lewis X mimetics as E-selectin inhibitors

INVENTOR(S): Wong, Chi-huey; Moris-Varas, Francisco; Lin, Chun-cheng; Marron, Thomas G.; Woltering, Thomas; Weitz-Schmidt, Gabriele; Jablonowski, Jill

PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Scripps Research Institute

SOURCE: PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

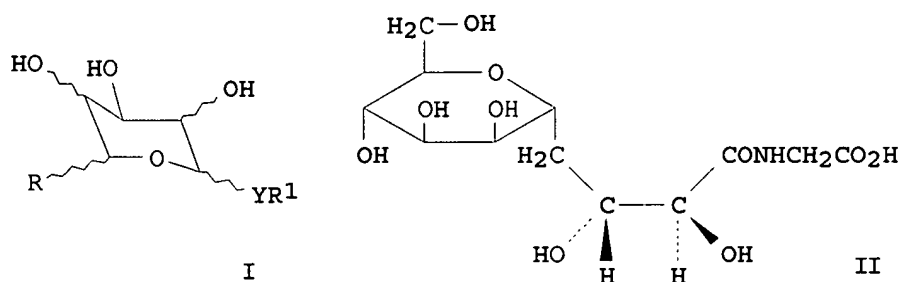
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9818805	A2	19980507	WO 1997-EP5909	19971027
WO 9818805	A3	20030417		
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW			
RW:	GH, KE, LS, MW, SD, SZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
US 5830871	A	19981103	US 1996-744744	19961028
US 5837862	A	19981117	US 1996-764315	19961212
AU 9853137	A1	19980522	AU 1998-53137	19971027
PRIORITY APPLN. INFO.:			US 1996-744744	A 19961028

US 1996-764315	A	199612 12
US 1997-896452	A	199707 18
WO 1997-EP5909	W	199710 27

OTHER SOURCE(S): MARPAT 129:4814  
GI



AB Sialyl Lewis X mimetics which mimic the inhibition of selectin-mediated cellular adhesion by sialyl Lewis X having a core of formula [(I); R = Me, OH, carboxylate-contg. sugar residue; Y = alkene; R1 = OH, NH2, amide, amino acid] were prepd. Thus, compds. such as II were prepd. and tested for ability to block the adhesion of HL-60 cells to immobilized sol-E-selectin. Compds. of formula I showed inhibition at 3mM of 70-80%, or IC50 values from 0.1-0.2mM.

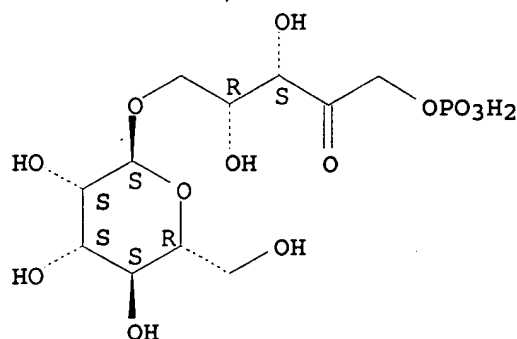
IT 194980-01-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of sialyl Lewis X mimetics as E-selectin inhibitors)

RN 194980-01-3 HCAPLUS

CN D-threo-2-Pentulose, 5-O- $\alpha$ -D-mannopyranosyl-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H015-00

CC 33-8 (Carbohydrates)

Section cross-reference(s): 34, 63

IT 186532-53-6P 186532-55-8P 186532-57-0P 186532-59-2P

186532-61-6P 194980-01-3P 194980-09-1P 194980-12-6P

194980-14-8P 204458-84-4P 204458-85-5P 204458-87-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of sialyl Lewis X mimetics as E-selectin inhibitors)

L17 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:163599 HCAPLUS

DOCUMENT NUMBER: 128:230633

TITLE: Preparation of sialyl Lewis x mimetics as E-selectin inhibitors

INVENTOR(S): Wong, Chi-Huey; Lin, Chun-Cheng; Woltering, Thomas J.; Marron, Thomas G.; Moris-Varas, Francisco; Jablonowski, Jill; Weitz-Schmidt, Gabriele

PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Scripps Research Institute; Wong, Chi-Huey; Lin, Chun-Cheng; Woltering, Thomas J.; Marron, Thomas G.; Moris-Varas, Francisco; Jablonowski, Jill; Weitz-Schmidt, Gabriele

SOURCE: PCT Int. Appl., 70 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

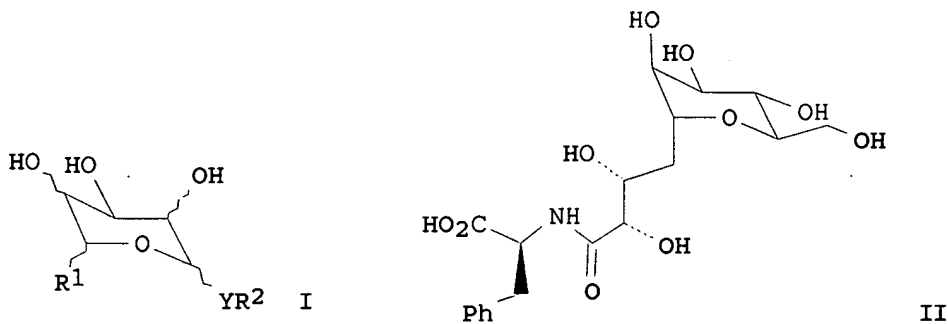
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9808854	A2	19980305	WO 1997-EP4649	19970826
WO 9808854	A3	19980820		

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU,

TJ, TM  
 RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI,  
 FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,  
 CM, GA, GN, ML, MR, NE, SN, TD, TG

US 5830871	A	19981103	US 1996-744744	199610 28
US 5837862	A	19981117	US 1996-764315	199612 12
AU 9747004	A1	19980319	AU 1997-47004	199708 26
PRIORITY APPLN. INFO.:			US 1996-24556P	P 199608 26
			US 1996-744744	A 199610 28
			US 1996-764315	A 199612 12
			WO 1997-EP4649	W 199708 26

OTHER SOURCE(S):           MARPAT 128:230633  
 GI



AB Sialyl Lewis X mimetics which mimic the inhibition of selectin-mediated cellular adhesion by sialyl Lewis X having a core of formula I (R<sub>1</sub> = Me, OH, carboxylate-contg. sugar residue; Y = alkylene; R<sub>2</sub> = hydroxy, amine, amide, amino acid) were prepd. Thus, II was prepd. and tested for ability to block the adhesion of HL-60 cells to immobilized sol-E-selectin (IC<sub>50</sub> = 0.1-0.2 mM).

IT 194980-01-3P

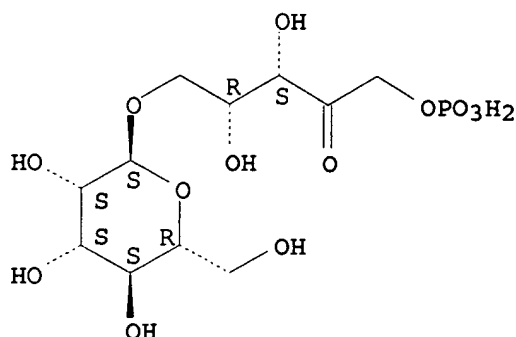
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (prepn. of sialyl Lewis x mimetics as E-selectin inhibitors)

RN 194980-01-3 HCAPLUS

CN D-threo-2-Pentulose, 5-O- $\alpha$ -D-mannopyranosyl-, 1-(dihydrogen

phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07H015-00

CC 33-8 (Carbohydrates)

Section cross-reference(s): 15, 34

IT 185753-18-8P 186532-53-6P 186532-55-8P 186532-57-0P  
 186532-59-2P 186532-61-6P 186585-85-3P 194980-01-3P  
 194980-02-4P 194980-09-1P 194980-12-6P 204458-75-3P  
 204458-76-4P 204458-78-6P 204458-80-0P 204458-84-4P  
 204458-85-5P 204458-87-7P 204458-89-9P

RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); BIOL  
 (Biological study); PREP (Preparation)  
 (prepn. of sialyl Lewis x mimetics as E-selectin inhibitors)

L17 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:667131 HCAPLUS

DOCUMENT NUMBER: 127:229196

TITLE: Small Molecules as Structural and Functional  
 Mimics of Sialyl Lewis X in Selectin Inhibition:  
 A Remarkable Enhancement of Inhibition by  
 Additional Negative Charge and/or Hydrophobic  
 Group

AUTHOR(S): Wong, Chi-Huey; Moris-Varas, Francisco; Hung,  
 Shang-Cheng; Marron, Thomas G.; Lin, Chun-Cheng;  
 Gong, Ke Wei; Weitz-Schmidt, Gabriele

CORPORATE SOURCE: Department of Chemistry, Scripps Research  
 Institute, La Jolla, CA, 92037, USA

SOURCE: Journal of the American Chemical Society (1997),  
 119(35), 8152-8158

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:229196

AB Several sialyl Lewis X (SLe<sup>x</sup>) mimics that contain the essential  
 functional groups for receptor interaction and a neg. charge or a  
 hydrophobic group have been developed as inhibitors of E-, P-, and  
 L-selectins. Some of the mimics exhibit selectin inhibition  
 activities 103-104-fold more potent than does the natural ligand  
 tetrasaccharide, with IC<sub>50</sub> in the low micromolar to high nanomolar  
 range. The syntheses of these mimics are relatively simple, using  
 TMSOTf-Ac<sub>2</sub>O mediated C-glycosylation with concurrent selective  
 deprotection of the primary benzyl group and enzymic aldol addn.

reactions as key steps.

IT 194980-01-3P

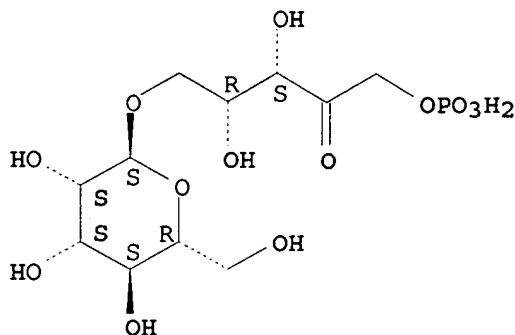
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(small mols. as structural and functional mimics of sialyl Lewis x in selectin inhibition in relation to addnl. neg. charge and/or hydrophobic Group)

RN 194980-01-3 HCAPLUS

CN D-threo-2-Pentulose, 5-O- $\alpha$ -D-mannopyranosyl-, 1-(dihydrogen phosphate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 1-3 (Pharmacology)

Section cross-reference(s): 33

IT 186532-57-0P 194980-01-3P 194980-02-4P 194980-09-1P

194980-12-6P 194980-14-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(small mols. as structural and functional mimics of sialyl Lewis x in selectin inhibition in relation to addnl. neg. charge and/or hydrophobic Group)

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:570752 HCAPLUS

DOCUMENT NUMBER: 111:170752

TITLE: Prokaryotic triterpenoids. A novel hopanoid from the ethanol-producing bacterium *Zymomonas mobilis*

AUTHOR(S): Flesch, Gerard; Rohmer, Michel

CORPORATE SOURCE: Ec. Natl. Super. Chim. Mulhouse, Mulhouse, 68093, Fr.

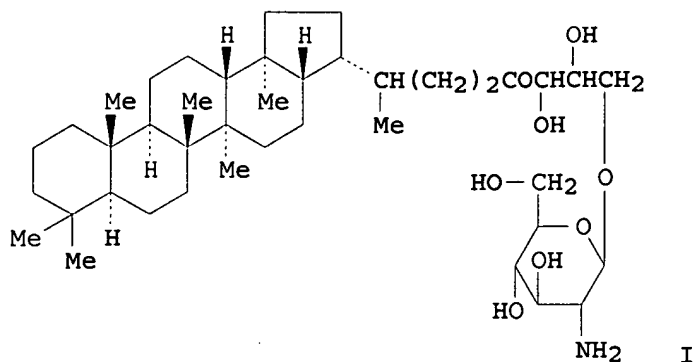
SOURCE: Biochemical Journal (1989), 262(2), 673-5

CODEN: BIJOAK; ISSN: 0306-3275

DOCUMENT TYPE: Journal

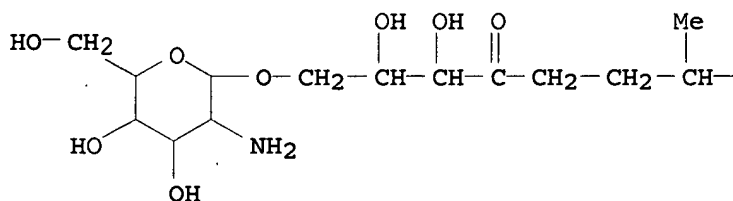
LANGUAGE: English

GI

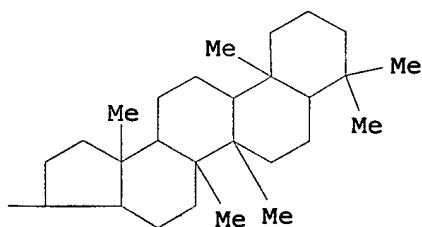


AB Among the triterpenoids of *Z. mobilis*, a novel hopanoid (I),  
 32-oxabacteriohopane-33,34,35-triol β-linked via its primary  
 hydroxy group to glucosamine, was isolated as a minor compd.  
 IT 123167-01-1  
 RL: BIOL (Biological study)  
 (from *Zymomonas mobilis*)  
 RN 123167-01-1 HCAPLUS  
 CN 4-Octanone, 1-[(2-amino-2-deoxy-β-D-glucopyranosyl)oxy]-2,3-  
 dihydroxy-7-[(21α)-A'-neo-22,29,30-trinorgammaceran-21-yl]-,  
 [2S-(2R\*,3R\*,7S\*)]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



CC 10-1 (Microbial Biochemistry)  
 Section cross-reference(s): 30

IT 123167-01-1  
RL: BIOL (Biological study)  
(from Zymomonas mobilis)

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